Simetone 673-04-1 | DTXSID9042388

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Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75	5%)	Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 2.61

Global applicability domain: Inside

Local applicability domain index: 5.15e-01

Confidence level: 6.75e-01

Nearest Neighbors from the Training Set

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Atraton

Measured: 2.69 Predicted: 2.94 Image not found

Simazine

Measured: 2.18 Predicted: 1.97

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Prometon

Measured: 2.99
Predicted: 3.01

Image not found

Trietazine
Measured: 3.34
Predicted: 3.32